Scattering theory of photon-assisted electron transport

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The scattering-matrix approach to phase-coherent transport is generalized to nonlinear ac transport. In photon-assisted electron transport it is often only the dc component of the current that is of experimental interest. But ac currents at all frequencies exist independently of whether they are measured or not. We present a theory of photon-assisted electron transport which is charge and current conserving for all Fourier components of the current. We find that the photocurrent can be considered as an up and down conversion of the harmonic potentials associated with the displacement currents. As an example explicit calculations are presented for a resonant double barrier coupled to two reservoirs and capacitively coupled to a gate. Two experimental situations are considered: in the first case the ac field is applied via a gate, and in the second case one of the contact potentials is modulated. For the first case we show that the relative weight of the conduction sidebands varies with the screening properties of the system. This is in contrast to the noninteracting case in which one finds that the relative weights are a universal function determined by Bessel functions. Moreover, interactions can give rise to an asymmetry between absorption and emission peaks. In the contact-driven case, the theory predicts at zero bias a photocurrent proportional to the asymmetry of the double barrier. [S0163-1829(98)03644-3]

I. INTRODUCTION

Photon-assisted tunneling has been of interest since the work of Tien and Gordon[1] and Tucker.[2] Carrier transmission through barriers with oscillating potentials has been analyzed to find the traversal time for tunneling.[3] Recently photon-assisted tunneling has found renewed interest in the field of mesoscopic physics stimulated by theoretical work by Bruder and Schoeller[4] and experiments on quantum dots by Kouwenhoven *et al.*,[5] and by experiments on superlattices by the group of Allen *et al.*[6–8] Typically of interest[4,5,7–24] is the zero-frequency current component induced in response to an oscillating voltage. Theoretical treatments of photon-assisted electron transport often assume that the driving field is known and equals the external field. However, the long-range Coulomb interaction will screen the external field and generates an internal potential that can be quite different from the applied potential. Similarly, since it is the dc component which is measured, one might think that displacement currents play no role. However, the dc component is a consequence of nonlinearities in the conduction process. Clearly, in such a conductor, the current has not only a dc component, but also currents at the frequency of the oscillating voltage and its higher harmonics. Not only are the dc currents conserved but also the currents at the oscillation frequency and at its higher harmonics. Consequently a theory is needed in which all frequency components of the current are treated self-consistently. Such a theory is developed below. It leads to the conclusion that the photocurrent is induced by a nonlinear up and down conversion of the electric fields (potentials) associated with the displacement current. Bessel functions are a hallmark[1] of the discussion of photon-assisted tunneling: For noninteracting theories the relative weights of the sideband peaks are determined by Bessel functions and are universal. However, in the self-consistent theory discussed below we find that the relative weights of the sideband peaks depend on the screening properties of the system. Since in nonstationary conditions charge accumulation occurs and causes induced fields, a self-consistent treatment of the electron-electron interactions is important. The issues are similar for theories and experiments which investigate photon-assisted process not in the dc current but in its fluctuations.[25,26] Here we emphasize mainly the average current and address the fluctuation spectra only briefly in the Appendix.

A convenient description of conduction processes in mesoscopic systems which incorporates the role of contacts and permits us to investigate directly the phase-coherent transmission from one reservoir to another, is the scattering-matrix approach.[27,28] The description of linear ac conduction in response to oscillating potentials and consideration of the long-range Coulomb interaction has already been discussed both for the case of zero-dimensional systems[29,30] and for extended systems for which one needs to discuss the entire potential landscape.[31,32] A review of this subject can be found in Ref. 33. Here we generalize the scattering-matrix approach to take into account the nonlinear dependence on oscillating potentials. First we consider the response of the electrons to a potential applied only to the contacts of the sample, assuming the internal potential is kept fixed. The response to the total potential will, in a subsequent step, be calculated self-consistently in random-phase-approximation (RPA). The resulting charge and current conserving theory will be used to investigate the photoinduced dc current in a resonant tunneling barrier. As function of Fermi energy and frequency we find large differences between the induced internal potential and the external applied potential, showing that long-range Coulomb forces are important for photon-assisted tunneling in mesoscopic systems. Furthermore, interactions can give rise to an asymmetry between absorption and emission peaks, as well as changing the distance between peaks from a multiple of photon quanta to a distance depending on screening properties.

Our discussion is complementary to works which model interactions based on a Hamiltonian suitable to describe Coulomb blockade effects. The work of Bruder and Schoeller[4] also considers coupling to a gate and also considers displacement currents. In principle, all the questions addressed here can be investigated within such a framework. The scattering approach used here has the advantage that it is not limited to the tunneling regime but can also be applied to conductors which are strongly coupled to reservoirs (ballistic or metallic diffusive wires, etc.). The RPA treatment as it is formulated below does have the disadvantage that it is not an appropriate description in the case when charge quantization effects (Coulomb blockade) are important. However, its conceptual clarity makes the RPA treatment a useful point of reference for comparison of different theoretical discussions.

The basic view taken here is the same as that used for the discussion of dc conductances[28] and ac conductance.[29] What is needed is the connection between currents at the contacts of the structure and the voltages at these contacts. Either the currents or the voltages can be controlled. As in the discussion of the ac conductance it is necessary to consider not only the mesoscopic conductor itself but all nearby metallic bodies (gates and capacitors) which interact via long-range Coulomb forces with the mesoscopic conductor. We assume that the conductor and the gates are connected to good quality metallic contacts in which screening is efficient. As a consequence the interior of the metallic contact is charge neutral. The electrostatic potential $U(\mathbf{r},t)$ and the electrochemical potential $\mu(t)$ oscillate in synchronism to keep the Fermi energy $E_F(\mathbf{r})=\mu(t)-eU(\mathbf{r},t)$ (the chemical potential) time independent. bA
voltage $V(t)$ applied to the contact
can thus be viewed both as a change in the electrochemical potential away from its equilibrium value or as a change in the conduction band bottom.[31] Let α label all the relevant contacts. The current at contact α can be written in terms of its Fourier components $I_\alpha(n\omega)$. Here $n=0$ is the dc component of the currents, and $n=\pm 1$ are the Fourier components at the driving frequency. Nonlinearities lead to higher harmonics $n=\pm 2,3,\ldots$. Similarly, the voltage at contact α has the Fourier components $V_\alpha(n\omega)$. We emphasize that the voltage of a contact is only a well defined quantity if local electric fields deep inside the contact vanish. There must, therefore, exist a Gauss volume which encloses the mesoscopic conductor.[29] The electric flux through this Gauss volume vanishes. As a consequence the total charge Q inside the volume is conserved.[29] Charge conservation, and current conservation, apply to each Fourier component separately. In particular, we must have that the total charge within the Gauss volume vanishes at each frequency,

$$Q_\alpha(n\omega)=0. \tag{1}$$

A theory for which this holds gives currents which depend ultimately only on voltage differences. We call such a theory of electric conductance gauge invariant.[34] To be definite let us introduce an expansion parameter ϵ. We take the Fourier components of the first harmonic $V_\alpha(\omega)$ proportional to ϵ and expand the currents in powers of ϵ. The second harmonic voltages $V_\alpha(2\omega)$ describing two-photon processes are then proportional to ϵ^2. Below we write the relationship between currents and voltages up to second order in ϵ. The expansion coefficients are conductances $g_{\alpha\beta\gamma}(n\omega,m\omega)$ which give the current at contact α in response to a voltage $V_\beta(n\omega)$ at contact β at a frequency $n\omega$ and a voltage a contact γ at a frequency $m\omega$. The overall dc current is

$$I_\alpha(0)=I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]+I_\alpha^{\mathrm{ph}}[0;\{V_\beta(0)\}], \tag{2}$$

$$I_\alpha^{\mathrm{ph}}[0;\{V_\beta(0)\}]=\sum_{\beta\gamma} g_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]V_\beta(\omega)V_\gamma^*(\omega). \tag{3}$$

The first term of Eq. (2), $I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]$, is the direct current that would be measured in the presence of purely static voltages $V_\beta(0)$, $\beta=1,2,\ldots$ applied to the different contacts of the sample and capacitors. In the following, for the direct current, we retain the full dependence to all orders in the static applied voltages. We indicated the full set of voltages with the help of curly brackets $V_\beta(0)$. If the dc current $I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]$ is expanded in powers of the applied voltage then the terms linear in the applied voltages determine the dc-conductance matrix $g_{\alpha\beta}(0)$ and the terms quadratic in the applied voltages are the dc-rectification conductances $g_{\alpha\beta\gamma}(0)$, discussed by Christen and one of the authors,[35,29] which determine the leading order nonlinearity of the dc I-V characteristic.[36] In addition to these contributions to the dc current which characterize the purely stationary transport there is now also a contribution to the dc current due to the photon-assisted processes, $I_\alpha^{\mathrm{ph}}[0;\{V_\beta(0)\}]$. In particular, to second order in the applied ac voltages $V_\beta(\omega)$, carriers which emit and reabsorb (virtual) photons are determined by the dc photoconductance $g_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]$ which depends in general also on the dc voltages $V_\delta(0)$. The first two arguments ω and $-\omega$ indicate the frequencies of the two driving voltages which give rise to this photoconductance. These photoconductance coefficients represent an up and down conversion of the first harmonic voltages.

The current at the frequency of the oscillating potential is in general composed both of a particle current and of a displacement current. To be brief we call this current simply the displacement current. To linear order in our expansion parameter it is given by

$$I_\alpha(\omega)=\sum_\beta g_{\alpha\beta}[\omega;\{V_\gamma(0)\}]V_\beta(\omega). \tag{4}$$

Here expanding $g_{\alpha\beta}[\omega;\{V_\gamma(0)\}]$ in the dc voltages yields the equilibrium admittance[30] of the mesoscopic structure $g_{\alpha\beta}(\omega)$ and the dc–ac rectification conductance $g_{\alpha\beta\gamma}(\omega;0)$.

The current at 2ω is

$$I_\alpha(2\omega)=\sum_\beta g_{\alpha\beta}[2\omega;\{V_\gamma(0)\}]V_\beta(2\omega) + \sum_{\beta\gamma} g_{\alpha\beta\gamma}[\omega,\omega;\{V_\delta(0)\}]V_\beta(\omega)V_\gamma(\omega) \tag{5}$$

determined by a second-harmonic conductance $g_{\alpha\beta}[2\omega;\{V_\gamma(0)\}]$ and a nonlinear up-conversion conductance $g_{\alpha\beta\gamma}[\omega,\omega;\{V_\delta(0)\}]$ whereby a second-harmonic current is generated due to a nonlinear combination of first-harmonic voltages. We emphasize that the expansion given

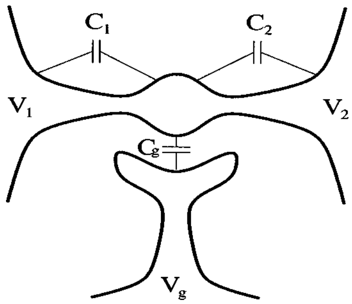

FIG. 1. Conductor connected to two contacts and coupled capacitively to a gate.

here can, in principle, be carried further to an arbitrary order in ϵ. Our task is to find explicit expressions for the (nonlinear) ac conductances defined in Eqs. (2)–(5). It is useful to state first a number of general properties of these conductances.

Current conservation holds for each Fourier component separately. Furthermore, since we can break off the expansion at any order, current conservation restricts each type of conductance coefficient in Eqs. (2)–(5). An additional restriction imposed on these conductance coefficients arises due to the fact that a voltage $V(n\omega)$ which is applied to all contacts simultaneously cannot have a physical effect. As a consequence the conductances obey the sum rules[35,29]

$$\sum_\alpha g_{\alpha\beta}(k\omega)=\sum_\beta g_{\alpha\beta}(j\omega)=0 \tag{6}$$

for $k,j\in\mathcal{N}$. Similarly, the second-order coefficients obey

$$\sum_\alpha g_{\alpha\beta\gamma}(k\omega,j\omega)=\sum_\beta g_{\alpha\beta\gamma}(k\omega,j\omega)=\sum_\gamma g_{\alpha\beta\gamma}(k\omega,j\omega)=0. \tag{7}$$

These sum rules guarantee that the final result will depend on voltage differences only.

Equations (2)–(5) are completely general and are applicable to any phase-coherent multiterminal conductor. We now discuss these general relations for the case of a two-terminal conductor capacitively coupled to a gate, a situation sketched in Fig. 1, in the limit $C_1=C_2=0$. This simple arrangement permits us already to point to the connection between photocurrents and displacement currents. We are interested in the photocurrent generated by a sinusoidal oscillation of the voltage $V_g(\omega)$ at the gate. First consider the displacement current. The oscillating gate couples with the conductor in a purely capacitive manner. Therefore, the $g_{\alpha g}[\omega;\{V_\beta(0)\}]$ describe capacitive currents and we can write $g_{\alpha g}[\omega;\{V_\beta(0)\}]=-i\omega C_{\alpha g}[\omega;\{V_\beta(0)\}]$. We emphasize that this is a global transport coefficient which connects the voltage at one contact to the current at another contact. As a consequence, the capacitance coefficients are not of a purely geometrical nature but can be strong functions of magnetic field and the dc gate voltage.[29,37,34,38] Thus, the current at contact α is determined by

$$I_\alpha(\omega)=-i\omega C_{\alpha g}[\omega;\{V_\beta(0)\}]V_g(\omega). \tag{8}$$

Next, consider the dc photocurrent generated by this arrangement

$$I_\alpha^{\mathrm{ph}}(0)=g_{\alpha gg}[\omega,-\omega;\{V_\beta(0)\}]|V_g(\omega)|^2. \tag{9}$$

Using Eq. (8) to eliminate the gate voltage $V_g(\omega)$ in Eq. (9) we find

$$I_\alpha^{\mathrm{ph}}(0)=\frac{1}{\omega^2}\frac{g_{\alpha gg}[\omega,-\omega;\{V_\beta(0)\}]}{|C_{\alpha g}[\omega;\{V_\beta(0)\}]|^2}|I_\alpha(\omega)|^2. \tag{10}$$

Thus to second order in the oscillating voltages, the photocurrent is directly related to the displacement current. The photocurrent is proportional to the square of the displacement current. This relation suggests that since the displacement current is not a property of a noninteracting system but is in an essential way determined by the long-range Coulomb interaction, so similarly, the long-range Coulomb interaction must play an essential role in determining the photocurrent. Note that the photoconductance which enters Eq. (10) is also proportional to ω^2 and the photocurrent given in Eq. (10) therefore has a well-defined zero-frequency limit. Now we proceed to find explicit expressions for the nonlinear conductances introduced above.

II. OSCILLATING CONTACT POTENTIALS: EXTERNAL RESPONSE

We consider a conductor with voltages which oscillate in time applied to the contacts of the sample or to nearby capacitors. First we evaluate the response of noninteracting particles with the internal potential kept fixed. Only the response to the total potential has physical meaning, however, these results are needed in the next section for treating the problem with interactions.

The current operator for current incident in contact α in a mesoscopic system can be written as[39]

$$\hat{I}_\alpha(t)=\frac{e}{h}\int dE\int dE'[\hat{\mathbf{a}}_\alpha^\dagger(E)\hat{\mathbf{a}}_\alpha(E')-\hat{\mathbf{b}}_\alpha^\dagger(E)\hat{\mathbf{b}}_\alpha(E')]e^{i(E-E')/\hbar t} \tag{11}$$

where $\hat{\mathbf{a}}_\alpha$ and $\hat{\mathbf{b}}_\alpha$ are vectors of operators with components $\hat{a}_{\alpha n}$ and $\hat{b}_{\alpha n}$. Here $\hat{a}_{\alpha n}$ annihilates an incoming carrier in channel n in lead α and $\hat{b}_{\alpha n}$ annihilates an outgoing carrier in channel n in lead α. Equation (11) applies for frequencies $(E-E')/\hbar$ small compared to the Fermi energy.

The incoming and outgoing waves are related by the scattering matrices[39] $\mathbf{s}_{\alpha\beta}$ via, $\hat{\mathbf{b}}_\alpha=\Sigma_\beta\mathbf{s}_{\alpha\beta}\hat{\mathbf{a}}_\beta$. In a multichannel conductor the matrix $\mathbf{s}_{\alpha\beta}$ has dimensions $N_\alpha\times N_\beta$ for leads with N_α and N_β channels. Here, and in the following, greek indices run over all contacts of the conductors.

Let us now suppose that a potential variation is applied to reservoir α. The potential is $eU_\alpha(t)=eV_\alpha(\omega)\cos\omega t$, where $V_\alpha(\omega)$ is the modulation amplitude. With this potential the solution to the single-particle Schrödinger equation at energy E in α is

$$\psi_{\alpha,n}(x,t;E)=\phi_{\alpha,n}(x;E)e^{-iEt/\hbar}\sum_{l=-\infty}^{\infty}J_l\left(\frac{eV_\alpha}{\hbar\omega}\right)e^{-il\omega t},\tag{12}$$

where $\phi_{\alpha,n}(x;E)$ is the wave function describing an incoming (or outgoing) carrier in contact α in channel n in the absence of a modulation potential, and J_l is the lth order Bessel function. Thus the potential modulation leads for each state with central energy E to sidebands at energy $E+l\hbar\omega$ describing carriers which have absorbed $l>0$ modulation quanta or have emitted $l<0$ modulation quanta $\hbar\omega$. Here we have assumed that all potentials oscillate in phase. If one allows for a different phase ϕ_α for each contact α that will add a term $e^{-il\phi_\alpha}$ to each term in the sum in the wave function above. Below, for simplicity, we assume that all contact potentials are in phase.

We now suppose that the modulation potential exists only far away from the conductor and that the modulation potential vanishes as we approach the conductor. Thus there is a transition region from a portion of the lead in which the potential is oscillating and a portion of the lead close to the conductor where we initially assume that the potential is time independent and equal to the equilibrium potential. We assume that in this transition region the potential varies slowly compared to the Fermi wavelength (adiabatic[40]) such that it does not give rise to additional scattering. Now we need the wave function in the time-independent potential region. This leads to a matching problem. If the transition is adiabatic a state with energy E in the conductor obtains a contribution from all reservoir states with central energy $E-l\hbar\omega$ due to its sideband of amplitude $J_l(eV_\alpha/\hbar\omega)$ at energy E. In the notation of second quantization the annihilation operator of an incoming state close to the conductor is

$$\hat{\mathbf{a}}_{\alpha,n}(E)=\sum_l \hat{\mathbf{a}}'_{\alpha,n}(E-l\hbar\omega)J_l\left(\frac{eV_\alpha}{\hbar\omega}\right),\tag{13}$$

up to corrections of the order of $\hbar\omega/E_F$ which arise from the difference of the wave vectors of the sidebands $p_l=\sqrt{2m(E+l\hbar\omega)}/\hbar$ and the wave vector at energy E. The current operator Eq. (11) is expressed in terms of the incoming (and outgoing) states of the stationary time-independent scattering problem. Equation (13) can now be used to find the current operator in terms of the reservoir states $\hat{\mathbf{a}}'_{\alpha,n}$. The current operator becomes

$$\hat{I}_\alpha(t)=\frac{e}{h}\int dE\int dE'\sum_{\gamma\delta}\sum_{lk=-\infty}^{\infty}(\hat{\mathbf{a}}')^\dagger_\gamma\times(E-l\hbar\omega)J_l\left(\frac{eV_\gamma}{\hbar\omega}\right)J_k\left(\frac{eV_\delta}{\hbar\omega}\right)e^{i(E-E')t/\hbar}\times\mathbf{A}_{\gamma\delta}(\alpha,E,E')\hat{\mathbf{a}}'_\delta(E'-k\hbar\omega),\tag{14}$$

where we have introduced the *current matrix*[39]

$$\mathbf{A}_{\delta\gamma}(\alpha,E,E')=\delta_{\alpha\delta}\delta_{\alpha\gamma}\mathbf{1}_\alpha-\mathbf{s}^\dagger_{\alpha\delta}(E)\mathbf{s}_{\alpha\gamma}(E').\tag{15}$$

It is assumed that the modulation imposed on the system is so slow that the contacts can still be regarded as being in a dynamic equilibrium state. Thus the quantum statistical average can be found by evaluating averages of the $\hat{\mathbf{a}}_\alpha(E-l\hbar\omega)$ as for an equilibrium system. Replacing the $\hat{\mathbf{a}}_\alpha(E-l\hbar\omega)$ by their equilibrium statistical expectation values we find

$$I_\alpha(t)=\frac{e}{h}\int dE\sum_{\gamma,lk}\mathrm{Tr}\,\mathbf{A}_{\gamma\gamma}(\alpha,E,E+(k-l)\hbar\omega)\times J_l\left(\frac{eV_\gamma}{\hbar\omega}\right)J_k\left(\frac{eV_\gamma}{\hbar\omega}\right)e^{-i(k-l)\omega t}f_\gamma(E-l\hbar\omega),\tag{16}$$

where $f_\gamma(E)=f(E-\mu_\gamma)$ is the Fermi distribution function for contact γ. Here μ_γ is the electrochemical potential of reservoir γ. In Eq. (16) the trace is over all channels in lead α. Taking into account the symmetry properties of the current matrix under exchange of the energy arguments it can be shown that the current given by Eq. (16) is real.

From Eq. (16) we find that for the dc current only the terms $l=k$ contribute. In this case, as is seen by looking at Eq. (16), the energy arguments of the current matrix are equal. The trace of the current matrix at equal energy arguments and equal lower lead indices are just transmission and reflection probabilities. We define $T_{\alpha\gamma}(E)=-\mathrm{Tr}\,\mathbf{A}_{\gamma\gamma}(\alpha,E,E)$. For unequal indices α and γ this is the transmission probability for carriers incident in lead γ to be transmitted into contact α. If also $\alpha=\gamma$ the trace of the current matrix is equal to the probability $R_{\alpha\alpha}$ of carriers incident in lead α to be reflected back into lead α, minus the number of quantum channels N_α at energy E. In this notation, particle conservation in the scattering process is expressed by the sum rule $\Sigma_\gamma T_{\alpha\gamma}=0$. For the dc current we find thus

$$I_\alpha(0)=-\frac{e}{h}\int dE\sum_{\gamma,l}T_{\alpha\gamma}(E)J_l^2\left(\frac{eV_\gamma}{\hbar\omega}\right)f_\gamma(E-l\hbar\omega).\tag{17}$$

Now we expand in this expression the Bessel functions in powers of the applied oscillating potentials V_γ. The zeroth-order terms give the dc current $I^{\mathrm{dc},(0)}[\{V_\beta\}]$ that flows as a consequence of stationary differences in the applied potentials. We use a superscript (0) to denote a response to an external potential only. Since the potential in the interior is kept fixed this I-V characteristic is not gauge invariant. A discussion is provided in Ref. 29 and by Christen and one of the authors.[35] The next term is second order in the amplitudes of the oscillating voltages. For identifying conductance coefficients recall that the applied potential is of the form $V_\gamma(t)=\frac{1}{2}V_\gamma(\omega)e^{i\omega t}+\frac{1}{2}V^*_\gamma(\omega)e^{-i\omega t}$, with the amplitudes taken as real. Thus, from the calculated response to $V_\gamma(t)$ we need to extract the response to the Fourier amplitudes. These second-order terms are determined by the photoconductances

$$g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]=-\delta_{\beta\gamma}\frac{e^3}{h}\int dE\,T_{\alpha\beta}[E;\{V_\delta(0)\}]\times\frac{f_\beta(E+\hbar\omega)+f_\beta(E-\hbar\omega)-2f_\beta(E)}{(\hbar\omega)^2}.\tag{18}$$

The photoconductance $g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]$ determines the zero-frequency current in contact α in response to a second-order voltage oscillation $V^2_\beta(\omega)$ at contact β. Note that the external photoconductance generated by bilinear products $V_\beta(\omega)V_\gamma(\omega)$ with β unequal to γ vanishes. Instead of a second-order difference in Fermi functions we can express the photoconductance as a second-order difference of transmission probabilities

$$g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega]=-\delta_{\beta\gamma}\frac{e^3}{h}\int dE f_\beta(E)\times\frac{T_{\alpha\beta}(E+\hbar\omega)+T_{\alpha\beta}(E-\hbar\omega)-2T_{\alpha\beta}(E)}{(\hbar\omega)^2}. \tag{19}$$

For simplicity we have not explicitly indicated the dependence on the stationary potentials $V_\delta(0)$. Equation (19) shows clearly that we obtain an externally induced photocurrent only if the transmission probabilities through the sample are energy dependent. Thus, for a quantum point contact or for a quantized Hall conductor, where we encounter situations characterized by transmission probabilities which are either zero or one, there is no externally induced photo current. This form of photoconductance also makes it evident that current conservation is satisfied due to the unitarity of the scattering matrix: The sum of all photoconductances over all contacts adds up to zero, $\Sigma_\alpha g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega]=0$. However, similar to the dc I-V characteristic these conductances are not gauge invariant. The sum $\Sigma_\beta g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega]$ does not vanish and consequently the photocurrent evaluated with these expressions depends not only on voltage differences.

Let us next consider the displacement current. The current at the frequency ω is determined by the terms in Eq. (16) for which $k-l=1$ and it is given by

$$I_\alpha(\omega)=\frac{e}{h}\int dE\sum_{\gamma,l}\mathrm{Tr}\,\mathbf{A}_{\gamma\gamma}(\alpha,E,E+\hbar\omega)\times J_l\left(\frac{eV_\gamma}{\hbar\omega}\right)J_{l+1}\left(\frac{eV_\gamma}{\hbar\omega}\right)f_\gamma(E-l\hbar\omega). \tag{20}$$

Linearizing the response to an oscillating external potential yields the admittance previously found.[29,30]

$$g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]=\frac{e^2}{h}\int dE\,\mathrm{Tr}\,\mathbf{A}_{\beta\beta}[\alpha,E,E+\hbar\omega;\{V_\gamma(0)\}]\times\frac{f_\beta(E)-f_\beta(E+\hbar\omega)}{\hbar\omega}. \tag{21}$$

The external admittance given by Eq. (21) has been the starting point of a self-consistent discussion of ac transport based on the scattering-matrix approach. The approach has been illustrated in a number of works.[42–44] The next term in the expansion is third order in the oscillating potentials and will not be needed here.

We remark that the external photoconductances Eq. (19) are like the dc current determined by transmission probabilities only. In contrast, the displacement current invokes products of scattering matrices at different energies and thus depends also on the phases of the scattering matrix. Expressed in a more physical language, the displacement current is sensitive to the densities of carriers, expressed here via energy derivatives of phases. Below we find that the self-consistent photocurrent contains in fact not only transmission probabilities but, like the displacement current, also information on the charge accumulated in the conductor.

Before considering the effect of screening, we discuss the relation of the external response to previous work. A discussion of shot noise in a conductor with applied ac voltages can be found in the Appendix.

A. Two-terminal conductors

We consider the external response for the two-terminal conductor. The conductor might consist of a single tunneling barrier or might be a resonant double barrier connected on either side to a large contact. The results we obtain from the external response described above look very similar to the results of Tien and Gordon[1] and Tucker.[2] There is, however, an important difference. The results presented in this section are not gauge invariant since in our approach the potential is held fixed also in the contacts near the barrier. As a consequence, different but physically identical configurations of voltages lead to different results. Later we will show how these results change when screening is taken into account, for the specific example of a resonant tunneling barrier. On the other hand, for a single barrier, as will be discussed briefly, the results by Tien and Gordon and Tucker do allow a gauge-invariant interpretation.

First we consider the zero-frequency photocurrent which arises if one of the contact potentials is oscillating and the other is kept fixed, $V_1(\omega)=V(\omega)$ and $V_2(\omega)=0$. For simplicity we assume that the scattering matrix has been diagonalized such that transmission through the barrier is described by a transmission probability $T_m(E)$ and a reflection probability $R_m(E)$ for the mth eigenchannel. Using Eq. (17) and using the sum rule for Bessel functions, $\Sigma_l J_{l+k}(x)J_l(x)=\delta_{k0}$, we find

$$I_1(0)=-\frac{e}{h}\int dE\sum_{lm}J_l^2\left(\frac{eV(\omega)}{\hbar\omega}\right)T_m(E)\times[f_1(E+l\hbar\omega)-f_2(E)]. \tag{22}$$

The time-dependent current was investigated by Tucker for the same geometry.[2] Using Eq. (16) we find

$$I_1(t)=\sum_{lk\gamma}\mathrm{Tr}\,\mathbf{A}_{\gamma\gamma}(\alpha,E,E+k\hbar\omega)\times J_l\left(\frac{eV(\omega)}{\hbar\omega}\right)J_{l+k}\left(\frac{eV(\omega)}{\hbar\omega}\right)e^{-ik\omega t}f_\gamma(E-l\hbar\omega). \tag{23}$$

Note that in contrast to the zero-frequency photocurrent the time-dependent current is expressed with the help of the current matrix, Eq. (15), and not with transmission probabilities. Neither Eq. (22) nor (23) is invariant under an equal shift of all potentials. For example, an experimentally equivalent situation would be to set $V_1(\omega)=V(\omega)/2$ and $V_2(\omega)=-V(\omega)/2$. This, however, yields a different result in the noninteracting approach. Even worse, setting $V_1(\omega)=V_2(\omega)=V(\omega)/2$ should yield no photocurrent, but gives the same as for $V_1(\omega)=V(\omega)/2$ and $V_2(\omega)=-V(\omega)/2$. To remedy this we introduce in the next section a simple self-consistent scheme to achieve charge and current conservation, similar to one used previously.[29,45]

The results of Tien and Gordon[1] and Tucker[2] have a slightly different appearance since the transmission probabilities are expressed with the help of Bardeen's formula $T=4\pi^2|t|^2\nu_1(E)\nu_2(E+l\hbar\omega)$ in terms of an energy-independent matrix element t and the density of states $\nu_1(E)$ and $\nu_2(E)$ to the left and right of the barrier. In our work the energy E is a global variable, whereas Tien and Gordon measure energy in the densities of states from the conduction band bottom to the left and right of the barrier. Of much more significance is the appearance of the voltage in their expressions and its meaning as compared to Eqs. (22) and (23). As explained by Büttner and Gerlach,[41] if one uses a coupling energy $e(V_1N_1+V_2N_2)\cos(\omega t)$ of the left and right contact voltages V_1 and V_2 to the total charges N_1 and N_2 of the left and right contacts and insists that $V=V_1-V_2$ is the experimentally applied voltage, then the tunneling Hamiltoian approach yields a gauge-invariant result which depends only on V. We remark here, that such a discussion only invokes the reservoir charges and reservoir potentials and does not attempt to provide a detailed description of the charge distribution near the barrier or inside a sample. Our approach is not restricted to such a minimal coupling of voltages and charges but in addition to the coupling of the contact voltages to the charges also treats the voltages and charges in the interior of the sample. To this extent we now proceed to the discussion of the charges injected into the sample.

B. Density operator

When applying voltages to the conductor, the sample will be charged. The net charge of the sample in response to a potential applied to a contact can be decomposed into two contributions: A charge response, called the injectance of the contact, at fixed internal electric potential and a charge response due to an electrically induced potential. Here we determined the injectances of a multiterminal conductor. In the next section these results are used when treating the problem with interactions.

At zero frequency, the number of electrons in the sample is determined by the operator[46]

$$\hat{N}=\sum_{\alpha\beta nm}\int d^2\mathbf{r}\int dE\,\nu_{\alpha n}^{1/2}(E)\nu_{\beta m}^{1/2}(E)\times\Psi_{\alpha n}^*(r,E)\Psi_{\beta m}(r,E)\hat{a}_{\alpha n}^\dagger(E)\hat{a}_{\beta m}(E), \tag{24}$$

where $\nu_{\alpha n}(E)$ is the density-of-states for channel n in contact α, and $\Psi_{\alpha n}(r,E)$ is the corresponding wave function for a scattering state describing carriers incident in contact α in channel n.

We now define the partial density-of-states matrix $d\mathcal{N}_{\alpha\beta}/dE$, with elements

$$\frac{d\mathcal{N}_{\alpha\beta,nm}}{dE}=\int d^2\mathbf{r}\,\nu_{\alpha n}^{1/2}(E)\nu_{\beta m}^{1/2}(E)\Psi_{\alpha n}^*(r,E)\Psi_{\beta m}(r,E). \tag{25}$$

This matrix can also be expressed in terms of the scattering matrix and its derivatives[46]

$$\frac{d\mathcal{N}_{\gamma\delta}}{dE}=-\frac{1}{4\pi i}\sum_\beta\left[\mathbf{s}_{\beta\gamma}^\dagger(E)\frac{d\mathbf{s}_{\beta\delta}(E)}{dE}-\frac{d\mathbf{s}_{\beta\gamma}^\dagger(E)}{dE}\mathbf{s}_{\beta\delta}(E)\right]. \tag{26}$$

Using this and Eq. (13) we find the number operator in the presence of oscillating contact potentials

$$\hat{N}=\sum_{\alpha\beta lk}\int dE\,J_l\left(\frac{eV_\alpha}{\hbar\omega}\right)J_k\left(\frac{eV_\beta}{\hbar\omega}\right)\times(\hat{\mathbf{a}}')_\alpha^\dagger(E-l\hbar\omega)\frac{d\mathcal{N}_{\alpha\beta}}{dE}\hat{\mathbf{a}}'_\beta(E-k\hbar\omega), \tag{27}$$

with the expectation value

$$N=\sum_{\alpha l}\int dE\,J_l^2\left(\frac{eV_\alpha}{\hbar\omega}\right)\mathrm{Tr}\frac{d\mathcal{N}_{\alpha\alpha}}{dE}f_\alpha(E-l\hbar\omega). \tag{28}$$

We can shift the frequency dependence from the Fermi function to the partial density of states

$$N=\sum_\alpha\int dE\,J_l^2\left(\frac{eV_\alpha}{\hbar\omega}\right)\frac{dN_\alpha^{(0)}}{dE}f_\alpha(E), \tag{29}$$

and thus identify the injectance $dN_\alpha^{(0)}/dE$ at energy E in the presence of a potential variation at contact α. Here the upper index 0 is once more used to emphasize that this density is evaluated at fixed internal potential. To second order in the oscillating potential, $V_\alpha(\omega)$, the injectance is

$$\frac{dN_\alpha^{(0)}}{dE}=\mathrm{Tr}\left[\frac{d\mathcal{N}_{\alpha\alpha}(E)}{dE}-\frac{e^2}{2}\frac{|V_\alpha(\omega)|^2}{(\hbar\omega)^2}\left(\frac{d\mathcal{N}_{\alpha\alpha}(E+\hbar\omega)}{dE}+\frac{d\mathcal{N}_{\alpha\alpha}(E-\hbar\omega)}{dE}-2\frac{d\mathcal{N}_{\alpha\alpha}(E)}{dE}\right)\right]. \tag{30}$$

In the limit that $|V_\alpha(\omega)|$ becomes small compared to $\hbar\omega$ the injectance is that produced by a static voltage. We have now determined both the currents and the charges as a consequence of oscillating voltages at the contacts of the sample under the assumption that the internal potential is kept fixed. We next determine the internal potential and the current and charge response to this internal potential.

III. INTERNAL RESPONSE: SELF-CONSISTENT SCREENING

In response to a potential variation at a contact the charge distribution in the interior of the sample is driven away from its equilibrium pattern. Coulomb interactions oppose such a variation. In the problem of interest here a variation of the sample charge can come about both because we in general consider a biased sample such that a dc current flows and because we subject the sample to ac voltages. In general it is a nonequilibrium dynamical potential landscape that matters. Here for simplicity we consider the sample to be zero dimensional and assume that it suffices to consider a single internal potential U. Such an approximation is often used in the literature on the Coulomb blockade and in the scattering approach to electrical conduction has been used to discuss the nonlinear I-V characteristic of mesoscopic samples[35] and ac transport in Refs. 45, 30, and 47. At equilibrium, if all voltages at the contact of the sample are equal, and in the absence of ac potentials, the value of this potential is $U=U_{\rm eq}$. Our first task is to determine the zero-frequency part of this potential.

To be more specific we now consider a sample coupled to a gate, as an example see Fig. 1. We denote the contact to the gate by the index g and the capacitance of the central region of the conductor to the gate by C_g. The capacitance between the central region of the conductor to the reservoir α is denoted by C_α. Next we introduce an index ν which runs over all N current contacts of the sample $\nu=\alpha=1,2,\ldots N$ and in addition includes the contact to the gate $\nu=N+1=g$.

A. Static internal potential

Consider first the equilibrium potential $U_0^{\rm eq}$. The grand canonical potential with the Coulomb energy included is minimal for a potential $U_0^{\rm eq}$ that obeys the Poisson equation. In our case the Poisson equation is discretized and is expressed with the help of the geometrical capacitances introduced above. The net electronic charge on the sample is that permitted by the Coulomb interaction:

$$Q-Q^+=\sum_\nu C_\nu(U-V_\nu). \tag{31}$$

Here Q is the electronic charge, Q^+ is an effective ''ionic charge'' created by the donors, and C_ν are the geometrical capacitances.

For $V_\nu=0$, the equilibrium charge $Q=Q_0^{\rm eq}$ and the equilibrium potential $U=U_0^{\rm eq}$ follow from Eq. (31) as follows. The electronic charge on the conductor can be expressed as a sum of all the charges injected from the various contacts,

$$Q_0^{\rm eq}=\sum_\alpha \int_{-\infty}^{\mu} e\frac{dN_\alpha(U_0^{\rm eq})}{dE}dE, \tag{32}$$

where the injectance[47,33] of contact α is given by Eq. (30). Note that the scattering matrix and thus the injectance also depends on $U_0^{\rm eq}$. Equation (32) is thus a self-consistent equation for the equilibrium potential.

Next, let us keep the ac voltages turned off but apply dc voltages to the contacts, charge will flow into the conductor causing a shift of the static potential in the barrier. We denote the resulting potential by U_0. It is a function of the applied potentials V_ν since now the injected charge depends on all the applied voltages. The injected charge is given by

$$Q_0=\sum_\alpha \int_{-\infty}^{\mu_\alpha} e\frac{dN_\alpha(U_0)}{dE}dE. \tag{33}$$

Using Eq. (32) to express the effective background charge in terms of the scattering matrix and the charges on the capacitors gives the following self-consistent equation for determining the internal static potential in the sample

$$\sum_\alpha \int_{-\infty}^{\mu_\alpha} e\frac{dN_\alpha(U_0)}{dE}dE-\int_{-\infty}^{\mu_{\rm eq}}\sum_\alpha e\frac{dN_\alpha(U_0^{\rm eq})}{dE}dE =\sum_\nu C_\nu(U_0-V_\nu). \tag{34}$$

Here $V_\alpha=\mu_\alpha-\mu$ is the deviation of the electrochemical potential in contact α from its equilibrium value μ. This approach was used by Christen and Büttiker[35] to study the nonlinear conductance for a resonant tunneling barrier.

Next, consider the case that is really of interest here. In addition to possible static voltage differences we have time-dependent potentials at the contacts. As a consequence the (unscreened) charge $Q(t)$ in the sample is also a function of time. It can be Fourier transformed, and we expect Fourier components at the oscillation frequency ω of the voltage and at all higher harmonics, $k\omega$. As a consequence the potential inside the conductor will also oscillate and will similarly have Fourier components at all harmonics, $U(k\omega)$. If an oscillating voltage at a contact, due to nonlinear processes, also changes the time-averaged charge in the sample then the potential U_0 as determined above would be modified by the presence of the oscillating potentials. To take this into account we write the injected charge as a response to external potentials in the presence of a self-consistently determined static potential plus the response from the internal oscillating potential. The response to the internal potential is determined by three unknown response coefficients, $\chi_{i\alpha}$, $\chi_{\alpha i}$, and χ_{ii} such that

$$Q_0=\sum_\alpha \int e\frac{dN_\alpha^{(0)}}{dE}dE+\sum_\alpha \int dE\chi_{i\alpha}(E)U^*(\omega)V_\alpha(\omega) +\sum_\alpha \int dE\chi_{\alpha i}(E)V_\alpha^*(\omega)U(\omega)+\chi_{ii}(E)|U(\omega)|^2. \tag{35}$$

To determine $\chi_{i\alpha}$, $\chi_{\alpha i}$, and χ_{ii} we use the fact that the injectance be invariant under a shift of all oscillating potentials by an equal amount. This yields the coefficients

$$\chi_{i\alpha}(E)=\chi_{\alpha i}(E) =\mathrm{Tr}\left[\frac{1}{2}\left(\frac{e}{\hbar\omega}\right)^2\left(\frac{d\mathcal{N}_{\alpha\alpha}(E+\hbar\omega)}{dE}+\frac{d\mathcal{N}_{\alpha\alpha}(E-\hbar\omega)}{dE} -2\frac{d\mathcal{N}_{\alpha\alpha}(E)}{dE}\right)\right], \tag{36}$$

$$\chi_{ii}(E)=-\sum_\alpha \chi_{i\alpha}(E). \tag{37}$$

With this we can express the gauge-invariant injectance as

$$\frac{dN_\alpha}{dE}=\mathrm{Tr}\left[\frac{d\mathcal{N}_{\alpha\alpha}(E)}{dE}-\frac{e^2}{2}\frac{|V_\alpha(\omega)-U(\omega)|^2}{(\hbar\omega)^2} \times\left(\frac{d\mathcal{N}_{\alpha\alpha}(E+\hbar\omega)}{dE}+\frac{d\mathcal{N}_{\alpha\alpha}(E-\hbar\omega)}{dE} -2\frac{d\mathcal{N}_{\alpha\alpha}(E)}{dE}\right)\right]. \tag{38}$$

Equations (34) and (38) now allow us to find the static internal potential U_0 in the presence of static and oscillating contact voltages. Note that dN_α/dE depends on U_0 since the scattering matrix depends on U_0. The potential U_0 depends on dc voltages applied to the sample and depends through nonlinear processes on the amplitudes of the ac voltages and the frequency. Our next task is now to find the *current* response to the oscillating internal potential $U(t)$.

B. dc current

Consider first the photoinduced dc current. The dc current can be divided into two parts, one due to direct transmission processes, and one due to transmission after absorption (emission) of a photon followed by its emission (absorption). Both processes take place in a self-consistently determined electrostatic background, which depends on all voltages at all frequencies:

$$I_\alpha(0)=I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]+I_\alpha^{\mathrm{ph}}[\{V_\beta(0)\}]. \quad (39)$$

Here $I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]$ is determined from the first term of the sum in Eq. (17), where now the scattering matrix depends on U_0.

The photocurrent can be written generally as the sum of the response to the external oscillating potential and the internal potential $U(\omega)$. To proceed we now consider $\epsilon = eU(\omega)/(\hbar\omega)$, a small parameter in which we can expand. All the oscillating contact potentials are also of order ϵ. In this work we will stop this expansion at the first nontrivial order. Since photon-assisted tunneling is of second or higher order in the oscillating potentials, we carry the expansion to second order.

For the photocurrent we obtain

$$\begin{aligned}I_\alpha^{\mathrm{ph}}[\{V_\beta(0)\}]=&\sum_{\beta\gamma} g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]V_\beta(\omega)V^*_\gamma(\omega)\\&+\sum_\beta g_{\alpha\beta i}[\omega,-\omega;\{V_\delta(0)\}]V_\beta(\omega)U^*(\omega)\\&+\sum_\gamma g_{\alpha i\gamma}[\omega,-\omega;\{V_\delta(0)\}]U(\omega)V^*_\gamma(\omega)\\&+g_{\alpha ii}[\omega,-\omega;\{V_\delta(0)\}]U(\omega)U^*(\omega), \quad (40)\end{aligned}$$

where the index i refers to responses due to the internal potential $U(\omega)$.

The responses to the internal potential are found by demanding that the current is invariant with respect to a shift of all voltages (gauge invariance). Lowering all voltages at frequency ω by $U(\omega)$ shifts the internal potential to the external potentials. Comparing the resulting expression with Eq. (40) gives

$$g_{\alpha\beta i}[\omega,-\omega;\{V_\delta(0)\}]=-\sum_\gamma g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}], \quad (41)$$

$$g_{\alpha i\gamma}[\omega,-\omega;\{V_\delta(0)\}]=-\sum_\beta g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}], \quad (42)$$

$$g_{\alpha ii}[\omega,-\omega;\{V_\delta(0)\}]=\sum_{\beta\gamma} g^{(0)}_{\alpha\beta\gamma}[\omega,-\omega;\{V_\delta(0)\}]. \quad (43)$$

Thus the photoresponses to the internal potential are determined by combinations of external photoconductances.

With these conductances, the dc current can be written as

$$I_\alpha(0)=I_\alpha^{\mathrm{dc}}[\{V_\beta(0)\}]+\sum_\beta g^{(0)}_{\alpha\beta\beta}[\omega,-\omega;\{V_\gamma(0)\}]|V_\beta(\omega)-U(\omega)|^2. \quad (44)$$

Note that the current depends on the difference between an applied voltage and the internal voltage only. All the nonlinear transport coefficients in Eqs. (40)–(44) also depend on U_0, the self-consistent dc potential.

C. Displacement current

The current at frequency ω is only needed to first order in the applied oscillating voltages. In addition to the external potential the oscillating internal potential also contributes to the current. In the presence of the internal potential the general form for the current is to first order in the potentials

$$I_\alpha(\omega)=\sum_\beta g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]V_\beta(\omega)+g_{\alpha i}[\omega;\{V_\gamma(0)\}]U(\omega). \quad (45)$$

Here $g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]$ are the external ac conductances given by Eq. (21) and $g_{\alpha i}$ is the ac response to the internal potential. Again we determine $g_{\alpha i}$ through the requirement that this expression is invariant under an overall shift of the potential. This gauge-invariance argument determines the response to the internal potential in terms of external responses; $g_{\alpha i}[\omega;\{V_\gamma(0)\}]=-\Sigma_\beta g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]$.

Both for the dc current and the ac current we now know the response to the external voltages $V_\gamma(0)$ and to the internal potential $U(t)$. But the internal potential is thus far not determined. This is our next task.

To be more specific we now return to the sample shown in Fig. 1. The current at contact α is the particle current plus the displacement current (capacitive) current $I_\alpha(\omega) - i\omega C_\alpha[V_\alpha(\omega)-U(\omega)]$ with I_α as determined above. The current from the gate to the sample is purely capacitive and is given by $I_g(\omega)=-i\omega C_g[V_g(\omega)-U(\omega)]$. Since the overall charge at frequency ω is conserved the sum of these currents must vanish. Thus we must have

$$\sum_\alpha I_\alpha(\omega)=-i\omega\sum_\nu C_\nu[U(\omega)-V_\nu(\omega)]. \quad (46)$$

Solving this equation for the internal potential yields

$$U(\omega)=\frac{\sum_{\alpha\beta} g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]V_\beta(\omega)-i\omega\sum_\nu C_\nu V_\nu(\omega)}{\sum_{\alpha\beta} g^{(0)}_{\alpha\beta}[\omega;\{V_\gamma(0)\}]-i\omega\sum_\nu C_\nu}. \quad (47)$$

The external ac conductances and the geometrical capacitances determine the potential $U(\omega)$ and determine the self-consistent dc current due to photoassisted tunneling and the self-consistent ac conductances.

IV. RESONANT TUNNELING BARRIER

As an application of the self-consistent theory developed above, we consider the photoinduced dc current through a resonant tunneling barrier. The experimental setup is taken as sketched in Fig. 1. Each side of the resonant barrier is connected to reservoirs with chemical potentials μ_1 and μ_2 and capacitances C_1 and C_2. The interior of the barrier is coupled to a gate with a capacitance C_g. For simplicity we assume that the gates are macroscopic with no dynamics of their own. A dc bias will be applied by making $eV \equiv e(V_1 - V_2) = \mu_1 - \mu_2$ nonzero.

The scattering matrix close to a resonance is given by the Breit-Wigner formula[48–50]

$$s_{mn} = \left[\delta_{mn} - i \frac{\sqrt{\gamma_m \gamma_n}}{E - E_0 - eU_0 + i\gamma/2} \right] e^{i(\delta_m + \delta_n)}. \tag{48}$$

Here γ_n, $n=1,2$ are the partial widths of the resonance proportional to the tunneling probability through the left and right barrier and $\gamma = \Sigma_n \gamma_n$ is the total width of the resonance. δ_m are the phases acquired in the reflection or transmission process and E_0 is the position of the resonance. The term $eU_0 = e[V_1(0) + V_2(0)]/2 + W$ ensures invariance upon a shift of the dc voltages.[35] W is determined by the conditions Eqs. (34) and (38), and is a function of $V_1(0) - V_2(0)$ only. The injectivities are[47]

$$\frac{dN_\alpha}{dE} = \frac{1}{2\pi} \frac{\gamma_\alpha}{(E - E_0 - eU_0)^2 + (\gamma/2)^2}. \tag{49}$$

The Breit-Wigner formula is a reasonable form for the scattering matrix as long as the energy does not get close to the next resonance level. Assuming that the level spacing of our system is large enough such that neighboring levels can safely be ignored we will use the formula in a wide energy range.

Photon-assisted tunneling is most easily seen either in the differential conductance as function of bias voltage $dI(V)/dV$, where side peaks show up at multiples of the photon energy, or in the dc current for small (infinitesimal) bias when varying the gate potential[5] $I(V_g)$. In Fig. 2 we show an example of a $dI(V)/dV$ curve using the noninteracting discussion, Eq. (22) and using the Breit-Wigner expression Eq. (48) with $U_0 = 0$. The potential of the left contact oscillates. We apply a dc voltage $V \equiv V_1 - V_2$, take $\hbar\omega/(\gamma/2) = 5$ and consider the symmetric case $\gamma_1 = \gamma_2 = \gamma/2$. In this and all the following examples we use $\epsilon^2 = 0.1$, for which the expansion to second order is pertinent. For this choice of parameters only the first sideband peaks can be resolved. In a noninteracting discussion one identifies $U_0 = V_g$ and as a consequence both the differential conductance as a function of dc voltage, or the current as a function of gate voltage, the sidebands are observed at a voltage corresponding to the photon energy. Discussions which neglect interactions do not discriminate between these two methods for observing photon-assisted transport. If we now consider the physically meaningful result, the theory which includes interactions, the general behavior will remain the same, but the two methods of analyzing photon-assisted transport, i.e., considering $dI(V)/dV$ or $I(V_g)$ now give in general different results. The effects brought about by screening, discussed in more detail in the next section, are: First, the relative weight of the sidebands and the central peaks will not be the same in the two situations. Second screening also brings about an asymmetry in the weights of the sidebands for $\pm n\hbar\omega$. In a discussion that neglects interaction the side bands have the same weight. In contrast, in the interacting case, if the equilibrium chemical potential does not coincide with the resonant energy, screening will be different for the two voltages where peaks are seen, and accordingly their weights will differ. Such asymmetries are seen in experiments.[7] Below we discuss these effects in detail.

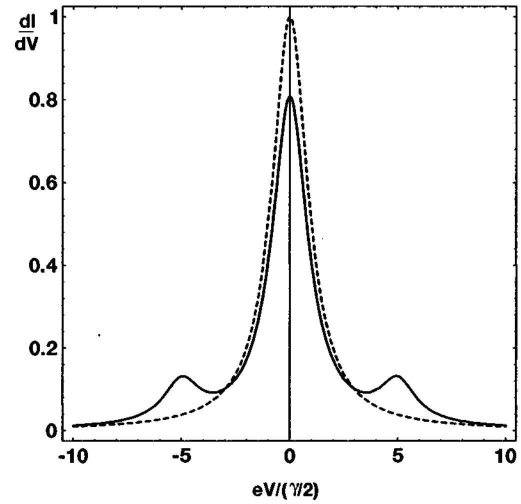

FIG. 2. Differential conductance as a function of dc bias from the noninteracting discussion. The left contact potential is oscillating. The parameters are $\hbar\omega/(\gamma/2) = 5$, $\epsilon^2 = 0.1$, and the Fermi energy is equal to the resonant energy $\mu = E_0$. For comparison the dashed line shows the transmission probability determined from the Breit-Wigner expression.

A. Gate-driven case

First, consider a sample subject to a dc bias $V = V_1 - V_2$ and an oscillating voltage $V_g(\omega)$ applied solely at the gate. For simplicity we take $C_1 = C_2 = 0$. In this case there can be no dc photocurrent when $\mu_1 = \mu_2$, since $\Sigma_\beta \mathbf{A}_{\beta\beta}(\alpha, E, E) = \mathbf{0}$ [see Eqs. (18) and (44)] as a consequence of the unitarity of the scattering matrix. The effect of photon-assisted tunneling in this setup is controlled by the internal potential. Thus, it is of interest to understand how it relates to the applied gate voltage in the presence of screening. From the self-consistent theory [see Eq. (47)] we find for the ratio of the applied to the external potential

$$\frac{U(\omega)}{V_g(\omega)}=\left[1+\frac{i}{\omega C}\sum_{\alpha\beta} g^{(0)}_{\alpha\beta}(\omega;V)\right]^{-1}. \tag{50}$$

This ratio is determined by the ac conductances $g^{(0)}_{\alpha\beta}(\omega;V)$. These ac conductances are known. At zero temperature, for the symmetric resonant tunneling barrier $\gamma_1=\gamma_2$ they are given by Fu and Dudley[51] and for the asymmetric case $\gamma_1\neq\gamma_2$ by Büttiker and Christen:[33]

$$g^{(0)}_{11}(\omega)=g^{(0)}_{21}(\omega)\left[\frac{\gamma_1}{\gamma_2}-\frac{\gamma}{\gamma_2}\left(1-i\frac{\hbar\omega}{\gamma}\right)\right], \tag{51}$$

$$g^{(0)}_{22}(\omega)=g^{(0)}_{12}(\omega)\left[\frac{\gamma_2}{\gamma_1}-\frac{\gamma}{\gamma_1}\left(1-i\frac{\hbar\omega}{\gamma}\right)\right], \tag{52}$$

$$g^{(0)}_{21}(\omega;V)=g^{(0)}_{12}(\omega;-V), \tag{53}$$

$$g^{(0)}_{12}(\omega)=\frac{e^2}{h}\,\frac{\gamma_1\gamma_2}{\gamma\hbar\omega}\,\frac{1}{1-i\,(\hbar\omega/\gamma)}\left[\frac{i}{2}\ln\frac{[(\mu-\hbar\omega-E_0-W-eV/2)^2+(\gamma/2)^2]}{[(\mu-E_0-W-eV/2)^2+(\gamma/2)^2]}+\frac{i}{2}\ln\frac{[(\mu+\hbar\omega-E_0-W-eV/2)^2+(\gamma/2)^2]}{[(\mu-E_0-W-eV/2)^2+(\gamma/2)^2]}\right.$$
$$\left.+\arctan\left(\frac{\mu+\hbar\omega-E_0-W-eV/2}{\gamma/2}\right)-\arctan\left(\frac{\mu-\hbar\omega-E_0-W-eV/2}{\gamma/2}\right)\right]. \tag{54}$$

With these expressions Eq. (50), the ratio of internal to external potential, can be evaluated. This ratio has two simple limits. In the noninteracting limit $C\to\infty$, the internal potential directly follows the applied potential. In the limit $C\to 0$, we have a charge neutral sample and $U(\omega)=0$.

In Fig. 3, we show the absolute square ratio of the internal to the external potential for different frequencies, when sweeping the Fermi level through the resonance. The non-screened case $C\to\infty$, where the ratio is 1, is shown as the dashed line. It is evident that screening introduces a large renormalization of the internal potential for this choice of capacitance with a strong dependence on frequency. One observes the largest effect when the Fermi energy is close to the resonance. This is expected since the density in the barrier is a Lorentzian with a peak at resonance,[48] thus providing more screening electrons. As a function of frequency the ratio changes qualitatively; for low frequencies the internal potential is reduced compared to the external potential, whereas with increasing frequency the situation reverses.

Next consider the current as a function of gate voltage. Since screening depends on the position of the resonant level compared to the equilibrium electrochemical potential, the central peak and the sideband will experience a different degree of screening and, thus, their weights will no longer be given by a Bessel function behavior as in the noninteracting approach. In Fig. 4 the ratio of the sideband peak to the

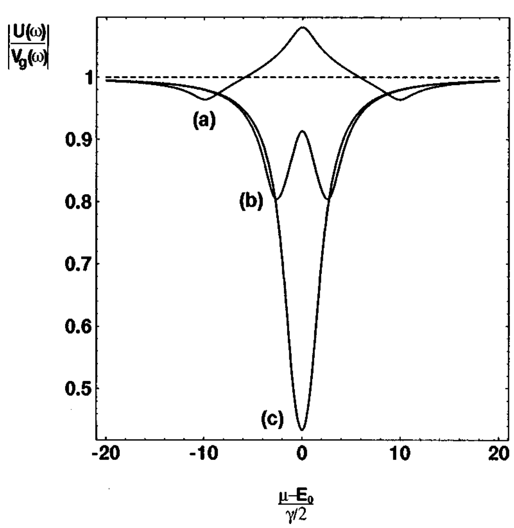

FIG. 3. Ratio of the internal potential to the gate voltage as function of the Fermi energy, for $C=e^2/\pi\gamma$, $V=0$ and for the frequencies (a) $\hbar\omega/(\gamma/2)=10$, (b) $\hbar\omega/(\gamma/2)=3$, and (c) $\hbar\omega/(\gamma/2)=1$.

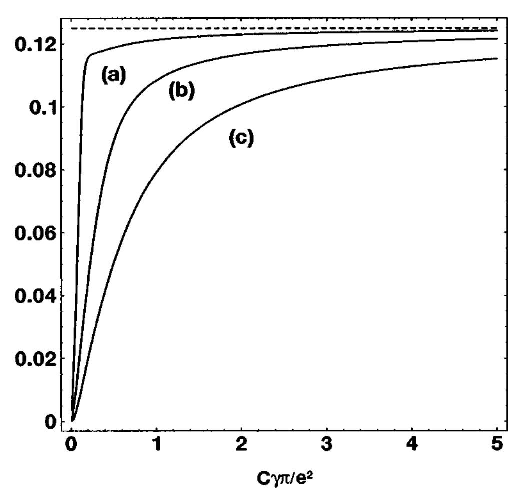

FIG. 4. Ratio of the sideband weight to central peak weight as function of capacitance in the current vs gate voltage characteristic $I(V_g)$ for frequencies (a) $\hbar\omega/(\gamma/2)=3$, (b) $\hbar\omega/(\gamma/2)=5$, and (c) $\hbar\omega/(\gamma/2)=10$, when $\epsilon^2=0.1$. The dashed line shows the result when no screening is present.

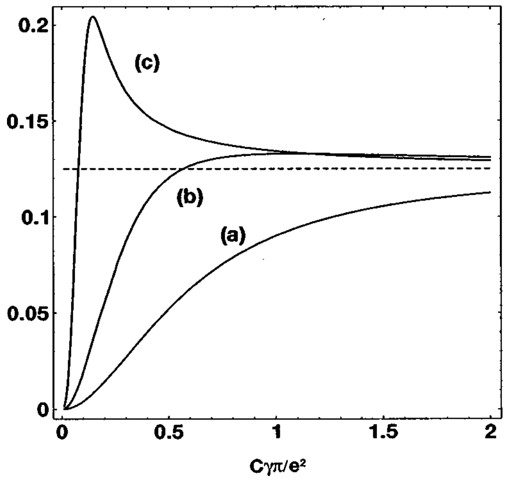

FIG. 5. Ratio of the sideband weight to the central peak weight as function of the capacitance in the differential conductance dI/dV for the frequencies (a) $\hbar\omega/(\gamma/2)=3$, (b) $\hbar\omega/(\gamma/2)=5$, and (c) $\hbar\omega/(\gamma/2)=10$ and $\epsilon^2=0.1$. The dashed line shows the result when no screening is present.

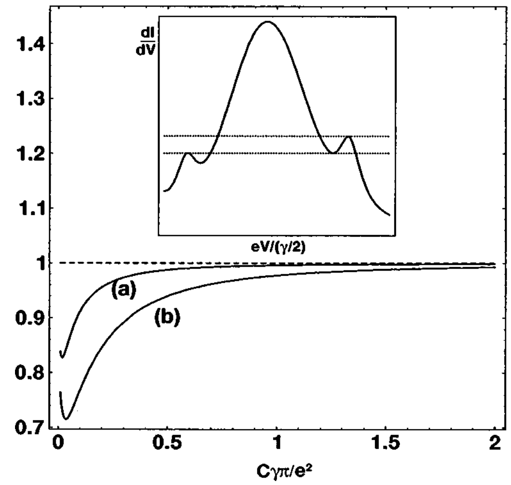

FIG. 6. Weight asymmetry for the $\pm\hbar\omega$ sidebands as function of capacitance in the dI/dV characteristic for $\gamma_1/(\gamma/2)=1/4$ and $\gamma_2/(\gamma/2)=3/4$, and for (a) $\hbar\omega/(\gamma/2)=3$, $\mu/(\gamma/2)=-5$, and (b) $\hbar\omega/(\gamma/2)=5$, $\mu/(\gamma/2)=-10$. The dashed line shows the result when no screening is present. The inset shows an example of a differential conductance curve as a function of the bias voltage for $\gamma_1=\gamma_2$, $\hbar\omega/(\gamma/2)=5$, $\mu/(\gamma/2)=-10$, and $C=0.1(e^2/\pi\gamma)$. The dashed line is the result without screening.

central peak is shown. The noninteracting approach predicts a ratio of 0.125 for the parameters chosen (dashed line). It is seen that, depending on capacitance and frequency, this ratio can be quite different.

Similarly, when measuring the differential conductance as function of dc voltage screening will also vary as function of voltage. In this case the sideband weight to central peak weight ratio is shown in Fig. 5. Again, large differences with respect to the noninteracting case are possible.

An interesting effect due to the dependence of screening on the dc voltage (or the gate voltage) is that sidebands will no longer be strictly Lorentzian, but skewed. However, this skewing effect is rather small and probably difficult to resolve experimentally.

When the Fermi level is off resonance the first sidebands corresponding to absorbing and afterwards emitting a photon and vice versa occur at different potentials. Screening will therefore occur asymmetrically for the two peaks introducing an asymmetry between the $\pm$ sidebands. This effect is illustrated in Fig. 6. Experimental observation of this effect has already been made,[7] although it has not been studied systematically.

Another effect is visible in the inset in Fig. 6. One notices that the width of the central peak is significantly larger than the width of the sidebands. Since the capacitance in this example is rather small, the charging energy is large, and when increasing the dc bias voltage the added charge gives rise to a huge increase in the static internal potential. The result is that the resonance floats upwards in energy, widening the peak. For the same reason, the distance from the central peak to the sideband is no longer simply $\hbar\omega$, but substantially larger.

B. Contact driven case

A setup often used experimentally is to couple the oscillating field to the conductor via a bowtie antenna.[7] In this case we assume that there is no gate, $C_g=0$. For simplicity we take the capacitances across each tunneling barrier to be identical, $C_1=C_2=C/2$. The dc current into contact 1 is then

$$I_1(0;V)=\left[g^{(0)}_{111}(\omega,-\omega;V)\left|\frac{\sum_\alpha g^{(0)}_{\alpha 2}(\omega;V)+i\omega C/2}{\sum_{\alpha\beta} g^{(0)}_{\alpha\beta}(\omega;V)-i\omega C}\right|^2 + g^{(0)}_{122}(\omega,-\omega;V)\left|\frac{\sum_\alpha g^{(0)}_{\alpha 1}(\omega;V)+i\omega C/2}{\sum_{\alpha\beta} g^{(0)}_{\alpha\beta}(\omega;V)-i\omega C}\right|^2\right] \times |V_2(\omega)-V_1(\omega)|^2. \tag{55}$$

In the absence of a dc voltage drop and for $\gamma_1=\gamma_2$, the dc photocurrent vanishes, because of the symmetry of the problem. However, in contrast to the gate driven case a zero-bias current can be generated for the asymmetric sample, given by

$$I_1(0;V=0)=g^{(0)}_{111}(\omega,-\omega)|V_2(\omega)-V_1(\omega)|^2\frac{\gamma_2-\gamma_1}{\gamma}\,\frac{|g^{(0)}_{12}(\omega)/\gamma_1\gamma_2|^2+\omega C[\mathrm{Re}\{g^{(0)}_{12}(\omega)\}/\gamma_1\gamma_2]}{|g^{(0)}_{12}(\omega)/\gamma_1\gamma_2-\omega C/\hbar\gamma|^2}. \tag{56}$$

Since $g_{12}^{(0)}(\omega)/(\gamma_1\gamma_2)$ is a function only of γ we find that the zero-bias current is proportional to the effective asymmetry of the double barrier, $(\gamma_1-\gamma_2)/\gamma$. For small capacitances, $C\gamma_1\gamma_2/(2\hbar g_{12}^{(0)}(\omega))\ll\gamma_1,\gamma_2$, the current is directly proportional to the asymmetry of the barrier without any renormalization from screening $I_1(0;V=0)=g_{111}(\omega,-\omega)|V_2(\omega)-V_1(\omega)|^2(\gamma_2-\gamma_1)/\gamma$. Thus, the ac field effectively pumps electrons through the system. The noninteracting result, given by Eq. (22), also predicts a current at zero bias. This result, however, being independent of the asymmetry of the system. This prediction of a zero-bias current for the symmetric case is again a consequence of the lack of gauge invariance of the noninteracting result. That a symmetric structure, in the absence of dc voltages, cannot exhibit a photocurrent, can be understood from the following symmetry and invariance conditions. Consider first a variation of the voltage at the left contact $V_1(\omega)=V_0\cos(\omega t)$ and suppose this produces a dc photocurrent I_1. Then consider a voltage variation of the right contact $V_2(\omega)=-V_0\cos(\omega t)=V_0\cos(\omega t+\pi)$. By symmetry this must give a current $I_2=-I_1$. In reality, however, due to gauge invariance these two voltage oscillations are experimentally the same and hence must give rise to the same dc current. But the only dc current which reflects this symmetry is $I=0$. Clearly, the correct answer is a consequence of gauge invariance.

V. CONCLUSION

We have extended the scattering-matrix approach to transport in phase-coherent conductors to take into account oscillating contact potentials and internal potentials in nonlinear order. The effect of screening has been taken into account to second order in the oscillating potentials by means of a RPA treatment. The result is a theory, valid for arbitrary dc voltages, which is current and charge conserving (gauge invariant). The internal potential in the conductor has been treated as a single parameter. Certainly, to go beyond this approximation and treat a more realistic continuous potential distribution would be interesting. But even for the case of linear ac transport, a scattering matrix for continuous potentials exists only to linear order in frequency,[31] and exceptionally to second order.[46] Discussions of the dynamic conductance of a ballistic wire over a wide range of frequencies, taking into account spatial potential variations,[32] are not yet formulated within the scattering approach. It would also be interesting to extend our discussion to higher order in the applied voltages. For large field strengths it is possible to make one of the Bessel functions zero, giving rising to dynamic localization.[52,8,12] Since we find that Bessel functions can in general not give a gauge-invariant answer it is clear that the criteria for dynamic localization will be changed in an essential way in the presence of interactions.

We have applied our theory to photon-assisted tunneling using a resonant tunneling barrier as an example. The two standard setups for photon-assisted tunneling, applying the modulation to one of the contacts in a two-terminal experiment, or coupling the potential to the conductor via a gate was examined within the self-consistent theory. In both cases, the inclusion of screening leads to a renormalization of the noninteracting answer. The driving field is not the applied field but the total field. Since the effective field is dependent on screening and therefore on applied bias, chemical potential, etc., the weights of the central peak and the side peaks in the differential conduction versus applied voltage differ from the noninteracting approach. Furthermore, the peak weight is no longer distributed according to the increasing order of Bessel functions. This leads to the peak ratios being a complicated function of the screening properties of the system. Experiments in single and double quantum dots show a rough qualitative agreement with the predictions of the noninteracting approach.[53] Quantitative comparisons between experiment and theory of the peak ratios are not available. The interacting theory also predicts an asymmetry between the corresponding left and right sidebands. Asymmetric photoconductance peaks have been observed.[7,5]

The necessity to include screening in the treatment of photoassisted transport is most clearly exemplified by the following consideration. For a spatially symmetric system a noninteracting approach predicts a photocurrent in response to the oscillation of either the left or the right contact voltage. In contrast, the gauge-invariant discussion presented here, predicts that a symmetrical system exhibits no photocurrent. Our result for the two-terminal resonant tunneling barrier, Eq. (56) is a photocurrent which is proportional to the asymmetry of the tunneling rates of the resonant double-barrier structure.

In this work we have emphasized that interaction effects are important whenever a variation of a parameter, an oscillation of a voltage, changes the charge away from its equilibrium value. In photoassisted tunneling it is not sufficient to consider just the dc current, but a theoretical discussion has to be self-consistent at all frequencies. Thus there is necessarily a relation between the photoassisted dc current and the displacement current. Only if the charge is investigated at all frequencies can an electrically meaningful, that is gauge invariant, answer be found.

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APPENDIX: CURRENT NOISE

The analysis of this paper concentrates on the average zero-frequency photocurrent. However, the approach used here also allows us to find the fluctuations of the current. Of particular interest are the current-current correlations which determine the spectral densities of the current fluctuations. Here we present the general result for the noise spectra of a multiterminal conductor in the presence of oscillating contact potentials assuming that the internal potential is kept fixed. As with the average dc current a physically meaningful result requires in general a discussion of the effects of screening.

For a multiprobe conductor with potentials $V_\alpha\cos(\omega t)$ at frequency ω applied to the contacts, using Eq. (14), we find the correlation function

$$\langle\{\Delta\hat{I}_\alpha(t+\tau),\Delta\hat{I}_\beta(t)\}\rangle=\left(\frac{e}{h}\right)^2\int dEdE'\sum_{\gamma\delta,lkl'k'}J_l\left(\frac{eV_\gamma}{\hbar\omega}\right)J_k\left(\frac{eV_\delta}{\hbar\omega}\right)J_{l'}\left(\frac{eV_\delta}{\hbar\omega}\right)$$
$$\times J_{k'}\left(\frac{eV_\gamma}{\hbar\omega}\right)e^{i(E-E')/\hbar\tau}e^{i(l+l'-k-k')\omega t}\mathrm{Tr}[\mathbf{A}_{\gamma\delta}(\alpha,E,E')\mathbf{A}_{\delta\gamma}(\beta,E'+(l'-k)\hbar\omega,E+(k'-l)\hbar\omega)]$$
$$\times[f_\gamma(E-l\hbar\omega)(1-f_\delta(E'-k\hbar\omega))+f_\delta(E'-k\hbar\omega)(1-f_\gamma(E-l\hbar\omega))]. \tag{A1}$$

Here the brackets $\{\}$ denote the anticommutator. In the presence of ac voltages the current-correlation function is not only a function of the relative time τ but depends also on the absolute time t. Experimentally what is of interest is the noise spectrum on a time scale long compared to $2\pi/\omega$. Therefore we define the noise spectrum as an average

$$S_{\alpha\beta}(\tau)=\frac{1}{2T}\int_0^T dt\,\langle\{\Delta\hat{I}_\alpha(t+\tau),\Delta\hat{I}_\beta(t)\}\rangle, \tag{A2}$$

where $T=2\pi/\omega$ is the period. The factor 1/2 arises because we have symmetrized the correlation function. The spectral density is related to the current-current correlation function via $2\pi S_{\alpha\beta}(\Omega;\omega)\delta(\Omega+\Omega')=(1/2)\langle\{\Delta\hat{I}_\alpha(\Omega),\Delta\hat{I}_\beta(\Omega')\}\rangle$, which is just the Fourier transform of $S(\tau)$. We find

$$S_{\alpha\beta}(\Omega;\omega)=\left(\frac{e}{\hbar}\right)^2\int dE\sum_{\gamma\delta,lkk'}J_l\left(\frac{eV_\gamma}{\hbar\omega}\right)J_k\left(\frac{eV_\delta}{\hbar\omega}\right)J_{k'+k-l}\left(\frac{eV_\delta}{\hbar\omega}\right)J_{k'}\left(\frac{eV_\gamma}{\hbar\omega}\right)\mathrm{Tr}[\mathbf{A}_{\gamma\delta}(\alpha,E,E+\hbar\Omega)\mathbf{A}_{\delta\gamma}(\beta,E+\hbar\Omega+(k'-l)\hbar\omega,E$$
$$+(k'-l)\hbar\omega)][f_\gamma(E-l\hbar\omega)(1-f_\delta(E+\hbar\Omega-k\hbar\omega))+f_\delta(E+\hbar\Omega-k\hbar\omega)(1-f_\gamma(E-l\hbar\omega))]. \tag{A3}$$

In the limit of vanishing driving frequency, $\omega=0$, Eq. (A3) reduces to the frequency-dependent noise spectra of Ref. 39.

For the special case that the scattering matrices can be taken to be independent of energy, i.e., $\mathbf{A}_{\gamma\delta}(\alpha,E,E+\hbar\omega)=\mathbf{A}_{\gamma\delta}(\alpha)$ Eq. (A3) simplifies considerably. Using the addition theorem for Bessel functions we find

$$S_{\alpha\beta}(0;\omega)=\left(\frac{e}{\hbar}\right)^2\int dE\sum_{\gamma\delta,l}\mathrm{Tr}[\mathbf{A}_{\gamma\delta}(\alpha)\mathbf{A}_{\delta\gamma}(\beta)]J_l^2\left(\frac{e(V_\delta-V_\gamma)}{\hbar\omega}\right)[f_\gamma(E+l\hbar\omega)(1-f_\delta(E))+f_\delta(E)(1-f_\gamma(E+l\hbar\omega))]. \tag{A4}$$

For a two-terminal conductor this result is identical to that of Lesovik and Levitov[25] even though in that work this result was derived in response to an electric field and not as here as a response to an oscillating contact voltage. In the experiment of Schoelkopf *et al.*[26] the shot noise is measured in the presence of an oscillating voltage applied to the contacts of the sample.

We emphasize that the noise spectra given by Eqs. (A3) and (A4) give only the noise for fixed internal potential. We have already remarked that the average dc current exhibits an external response due to photon-assisted transport only if the transmission probabilities exhibit an energy dependence [see Eq. (19)]. In contrast, in the shot-noise spectra, we have an effect even if the scattering matrix is taken to be energy independent. That is a consequence of the fact that the noise spectra depend in a nonlinear way on the Fermi functions.

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